

Supporting Information:

Molecular Design of Anticancer Drug from Marine Fungi Derivatives

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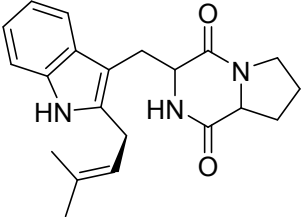
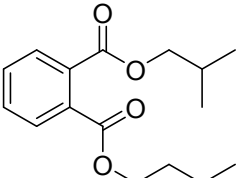
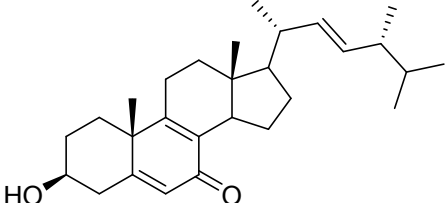
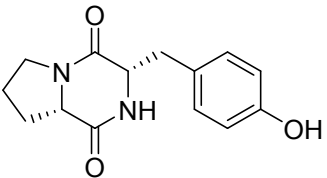
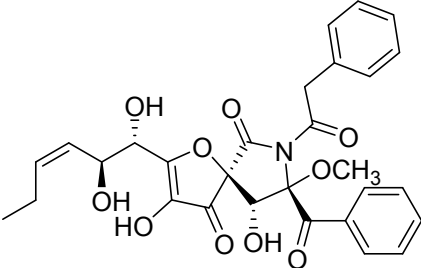
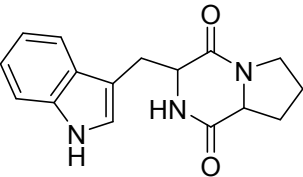
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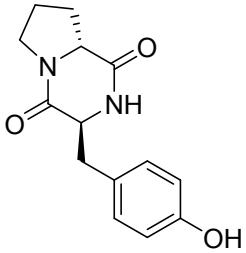
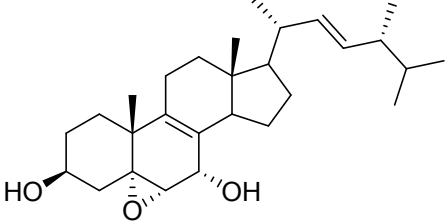
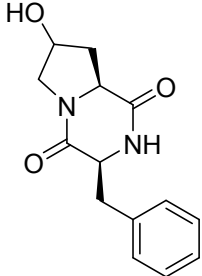
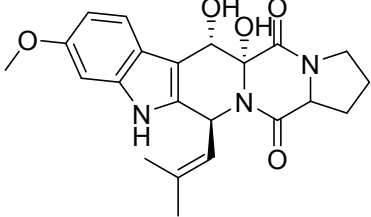
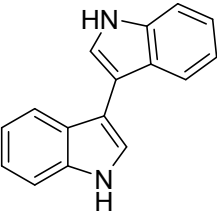
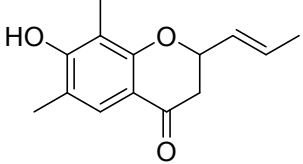
^dCollege of Pharmacy, Chungnam National University, Daejeon, Republic of Korea

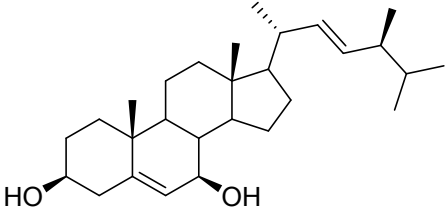
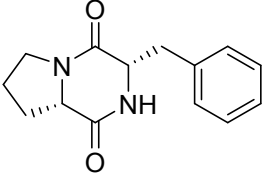
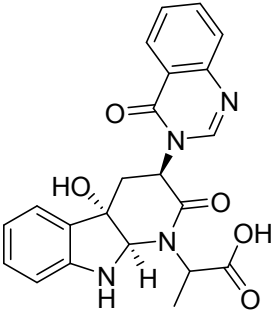
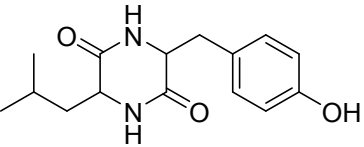
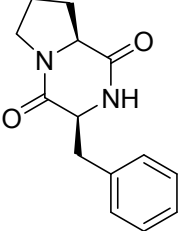
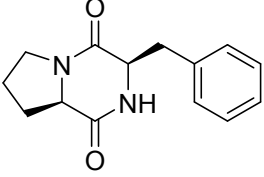
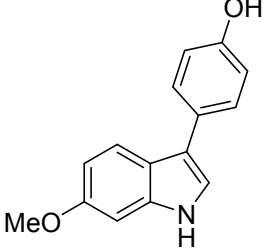
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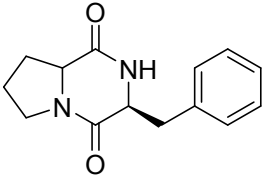
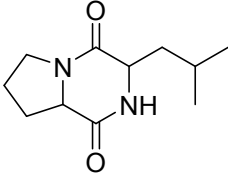
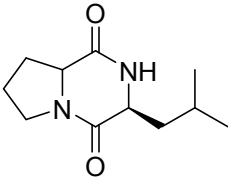
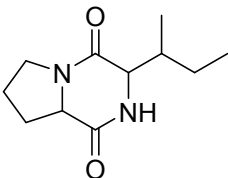
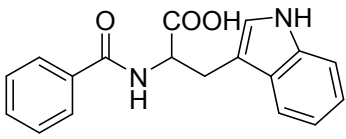
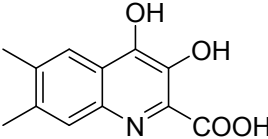
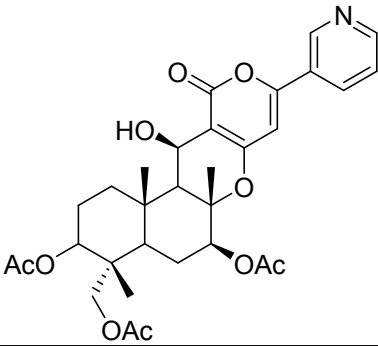
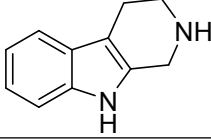
Email: nvhung@hpmu.edu.vn and minhquanaries@gmail.com

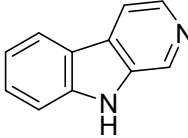
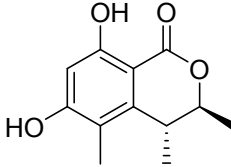
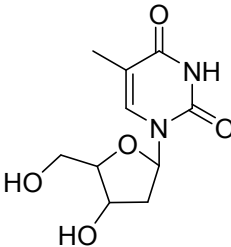
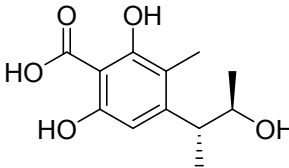
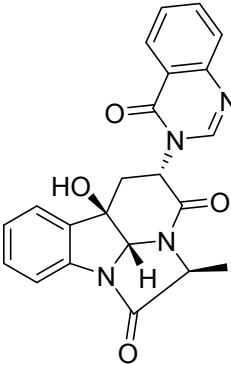
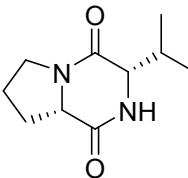
Table S1. The list of marine compounds and docking results.

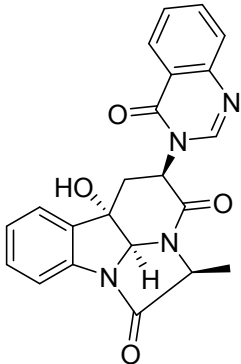
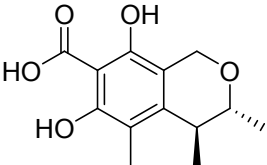
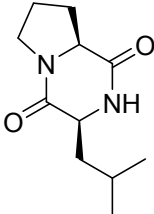
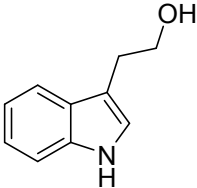
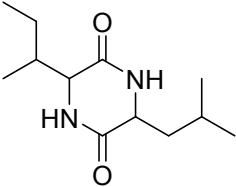
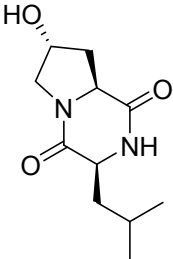
N ^o	ID	Structure	ChemPLP
1	48		86.33
2	25		77.8
3	40		76.9
4	23		72.58
5	46		71.73
6	52		70.55

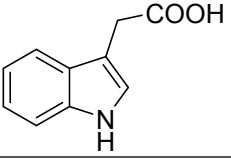
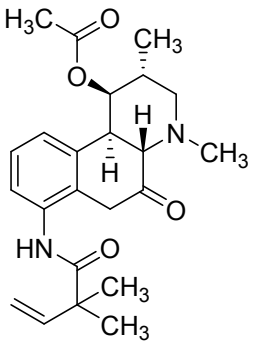
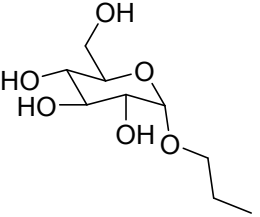
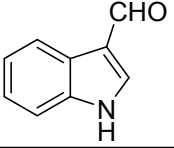
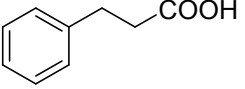
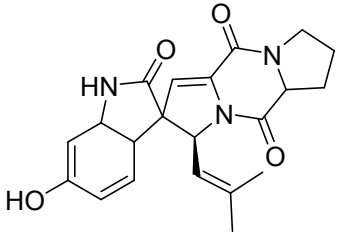
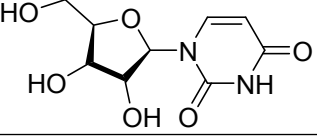
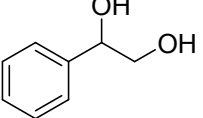
7	3	 <chem>Oc1ccc(cc1)CC2C(=O)NCC2=O</chem>	68.9
8	41	 <chem>CC(C)C=C[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C</chem>	68.61
9	1	 <chem>O[C@@H]1CCN(C1)C(=O)C2=CC=CC=C2</chem>	67.97
10	45	 <chem>COc1ccc2c(c1)c3c(c2)nc4c3c5c(c4)nc(=O)n5</chem>	67.45
11	13	 <chem>C1=CC=C2C(=C1)N=C(C2)c3c[nH]c4ccccc34</chem>	67.1
12	35	 <chem>CC1=C(O)C(=O)OC(=C1)C=C</chem>	67.05

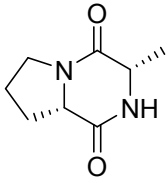
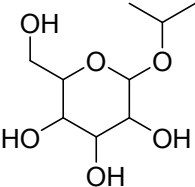
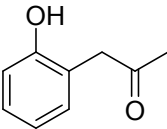
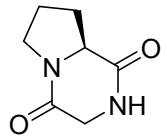
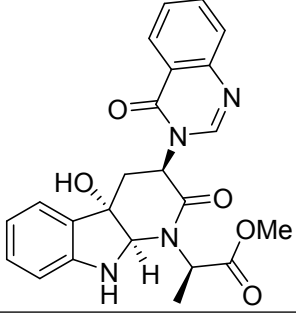
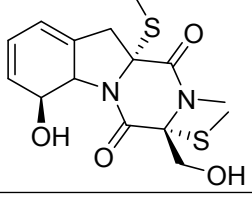
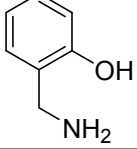
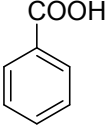
13	6	 <chem>CC(C)C=C[C@H](C)C[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C</chem>	66.49
14	22	 <chem>C1CCN(C1)C(=O)N[C@@H](C1=CC=CC=C1)C(=O)N1CCCC1</chem>	66.32
15	MG12	 <chem>CC(C)C(O)N1C(=O)N(C1)C(=O)N2C(=O)N(C2)C3=CC=CC=C3</chem>	65.3
16	29	 <chem>CC(C)C(=O)N[C@@H](C)C(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)N</chem>	64.69
17	4	 <chem>C1CCN(C1)C(=O)N[C@@H](Cc2ccccc2)C(=O)N1CCCC1</chem>	64.47
18	21	 <chem>C1CCN(C1)C(=O)N[C@@H](Cc2ccccc2)C(=O)N1CCCC1</chem>	64.01
19	MG5	 <chem>COc1ccc2c(c1)c(c[nH]2)C3=CC=C(O)C=C3</chem>	62.84

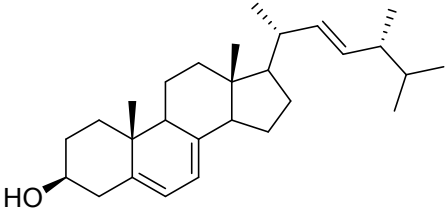
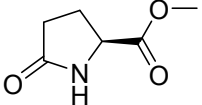
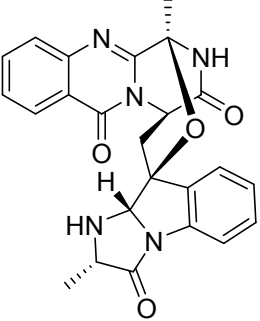
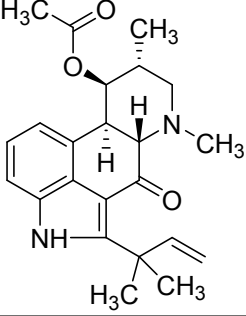
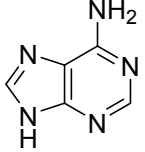
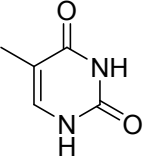
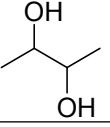
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21	19		61.82
22	51		61.37
23	20		60.74
24	MG10		59.65
25	9		59.2
26	MGA 2		58.99
27	MG7		58.38

28	14	 <chem>Cc1ccc2c(c1)c(c[nH]2)c3cccnc3</chem>	57.8
29	36	 <chem>Cc1cc(O)c(O)c(c1)C[C@H](O)C(=O)O</chem>	57.52
30	42	 <chem>Cc1cc(O)c(O)c(c1)C[C@H](O)C(=O)N1C(=O)C(=O)N1</chem>	57.51
31	38	 <chem>Cc1cc(O)c(O)c(c1)C[C@H](O)C(=O)O</chem>	57.39
32	MG2-1	 <chem>Cc1c2c(c3c1c[nH]3)C(=O)N2C(=O)N1C(=O)C(=O)N1</chem>	57.04
33	18	 <chem>Cc1c2c(c3c1c[nH]3)C(=O)N2C(=O)N1C(=O)C(=O)N1</chem>	56.47

34	MG4-1		56.12
35	37		55.73
36	5		55.45
37	7		55.36
38	28		55.16
39	2		55.08

40	11		54.68
41	MGA 1		53.36
42	33		53.07
43	10		52.24
44	12		52.21
45	47		50.8
46	MG1		50.77
47	16		50.49

48	17		50.33
49	34		50.24
50	24		50.18
51	8		49.38
52	MG4-2		47.87
53	44		46.2
54	26		45.88
55	15		44.32

56	39	 <chem>CC(C)C(C)C=C[C@H](C)C[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C</chem>	42.06
57	49	 <chem>COC(=O)[C@H]1CC(=O)N1</chem>	41.01
58	43	 <chem>C[C@H]1NC(=O)[C@@H]2[C@@H](C1)N(C(=O)N2)c3ccccc3</chem>	40.7
59	MG8	 <chem>CC(=O)OC[C@H]1[C@@H](C)N(C)[C@@H]2[C@@H](C1)C(=O)N=C2C</chem>	40.41
60	31	 <chem>NC1=NC=NC2=C1N=CN2</chem>	37.44
61	32	 <chem>CC1=CN(C(=O)N1)C(=O)N</chem>	36.19
62	27	 <chem>CC(O)C(C)O</chem>	32.1

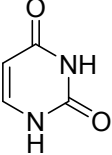
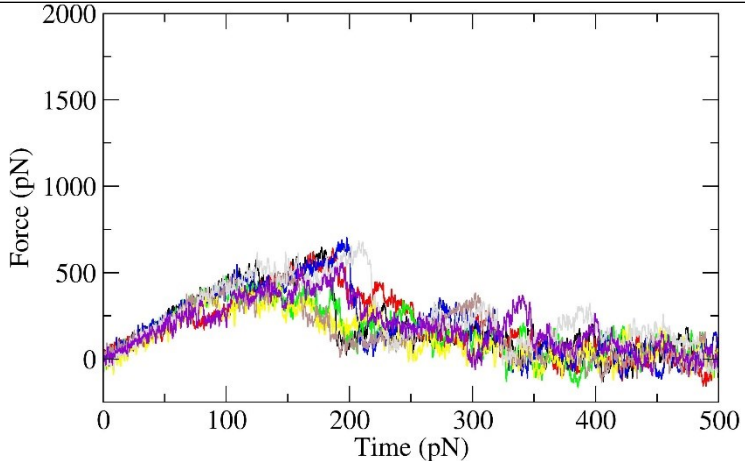
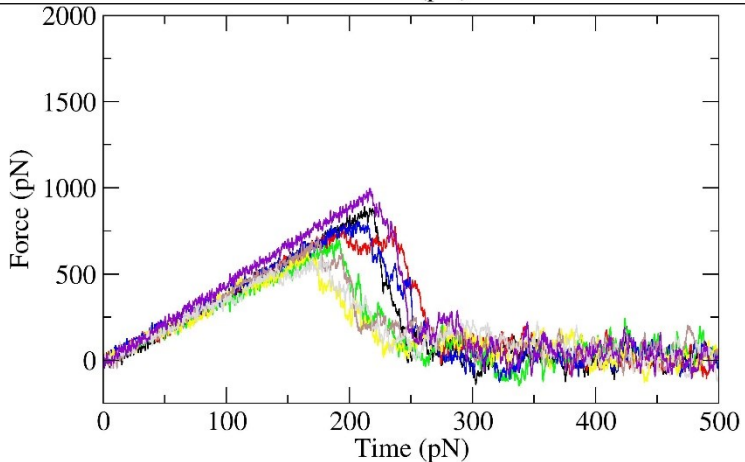
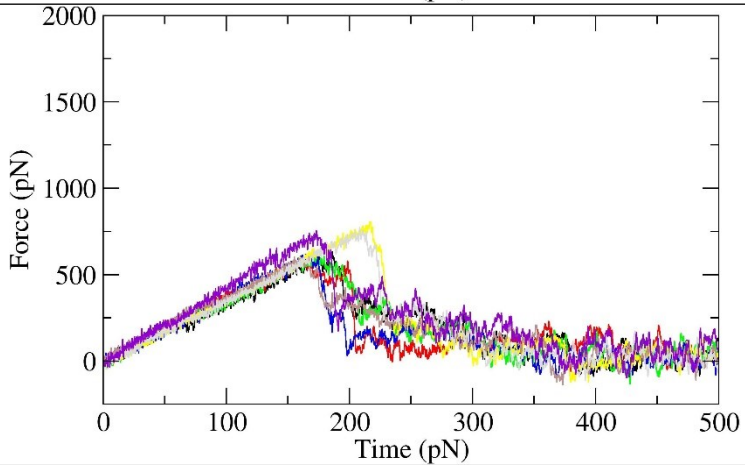
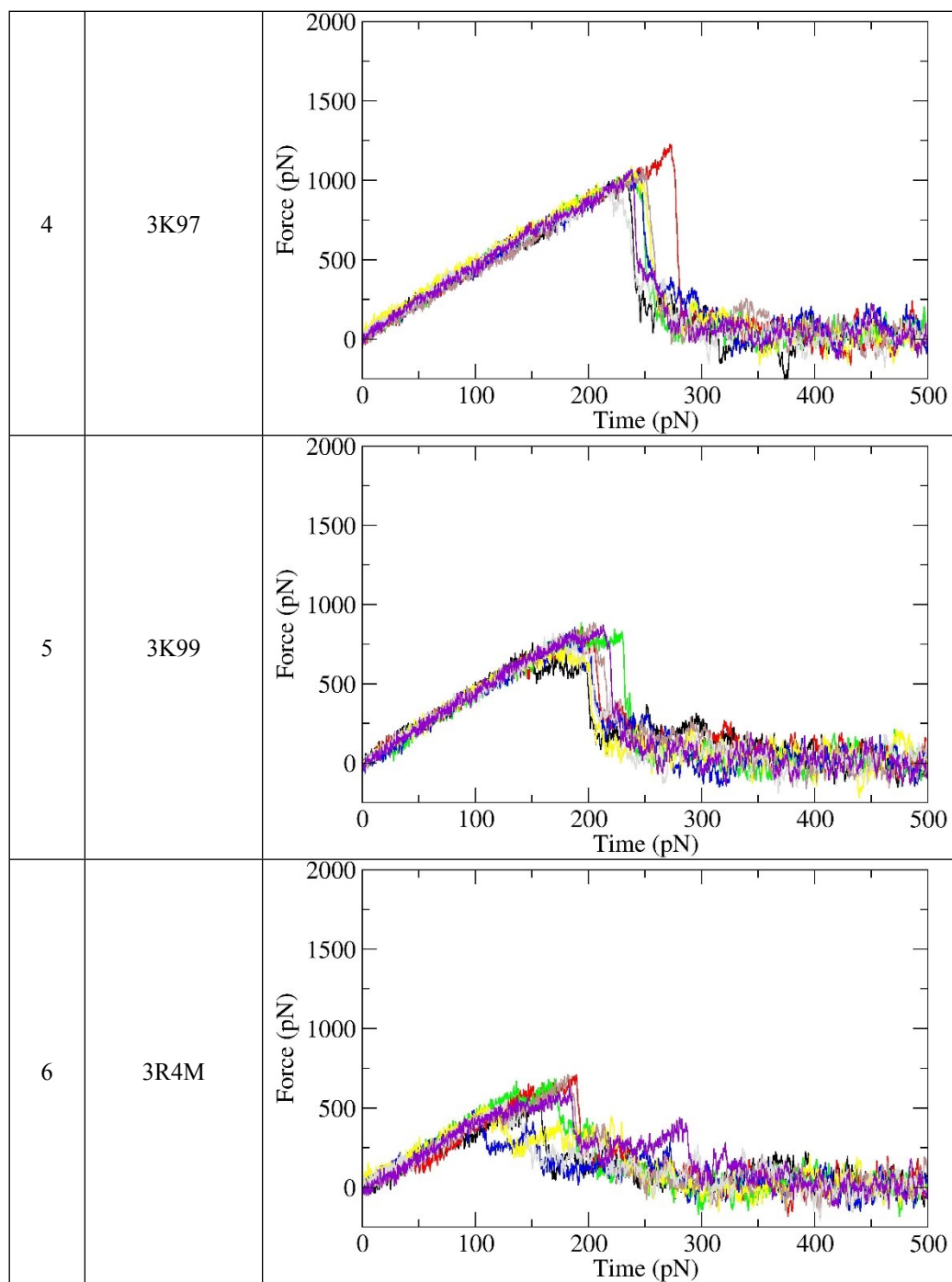
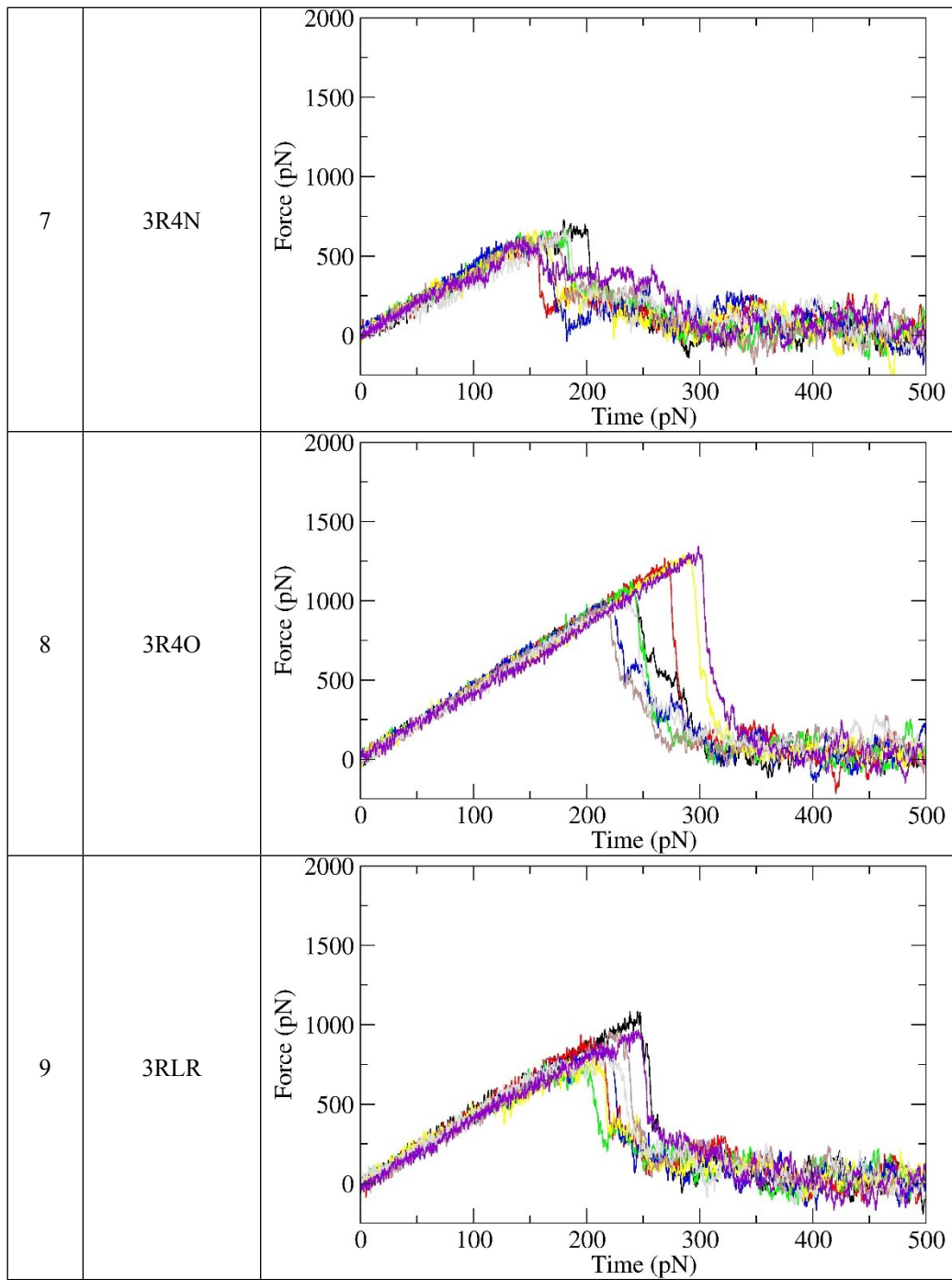
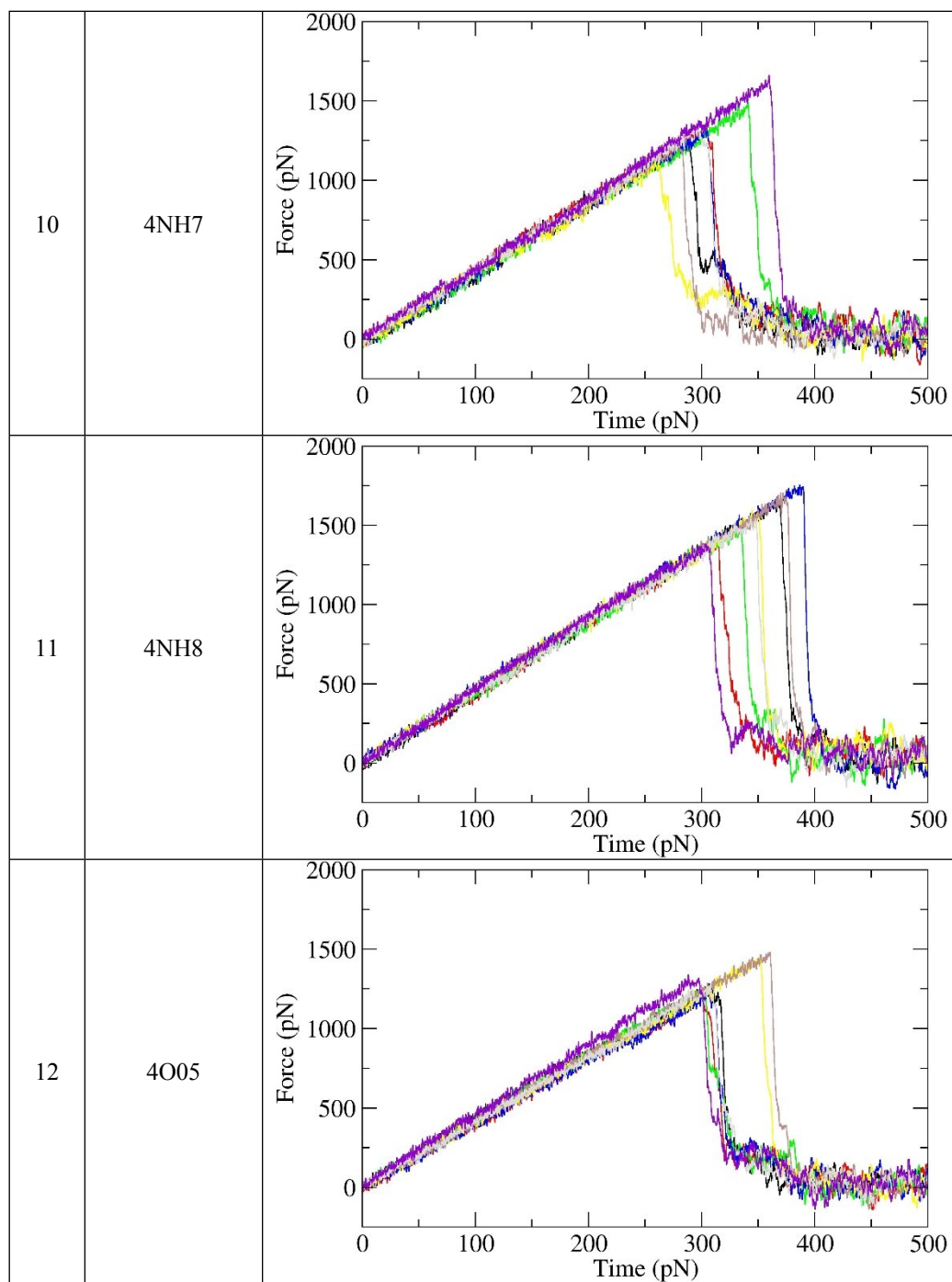
63	30	 <chem>C1=CN(C(=O)N1)C=O</chem>	31.99
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Table S2. The list of available inhibitors and FPL results.

N ^o	PDB ID	Pulling Work
1	2QF6	 A line graph showing Force (pN) on the y-axis (0 to 2000) versus Time (pN) on the x-axis (0 to 500). Multiple colored lines represent different pulling work trials. The force increases from 0 to approximately 500 pN at 100 pN time, reaches a peak of about 600 pN at 200 pN time, and then drops to near 0 pN by 300 pN time, remaining low until 500 pN time.
2	2QG0	 A line graph showing Force (pN) on the y-axis (0 to 2000) versus Time (pN) on the x-axis (0 to 500). Multiple colored lines represent different pulling work trials. The force increases from 0 to approximately 700 pN at 100 pN time, reaches a peak of about 1000 pN at 200 pN time, and then drops to near 0 pN by 300 pN time, remaining low until 500 pN time.
3	2QG2	 A line graph showing Force (pN) on the y-axis (0 to 2000) versus Time (pN) on the x-axis (0 to 500). Multiple colored lines represent different pulling work trials. The force increases from 0 to approximately 500 pN at 100 pN time, reaches a peak of about 700 pN at 200 pN time, and then drops to near 0 pN by 300 pN time, remaining low until 500 pN time.







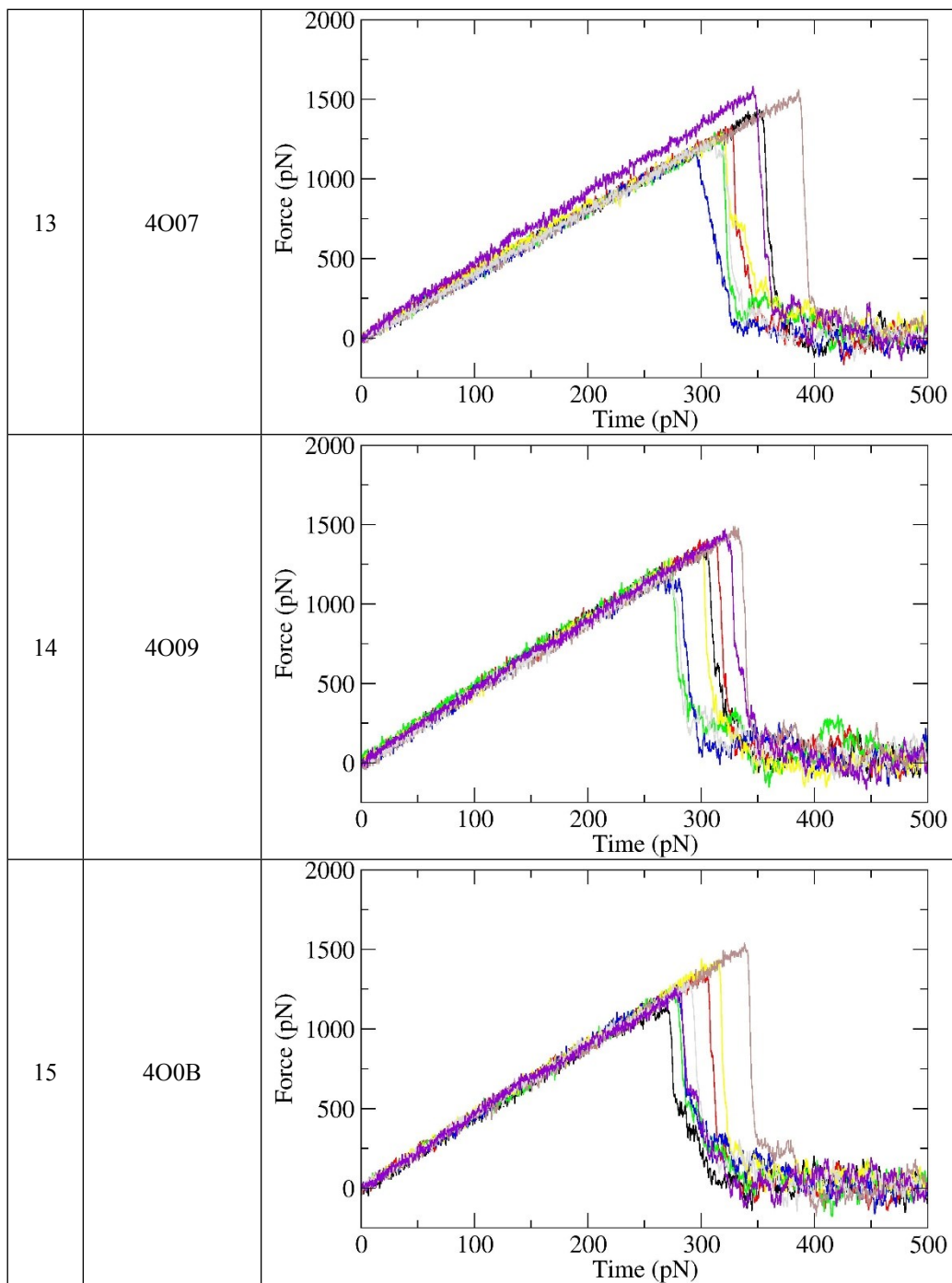
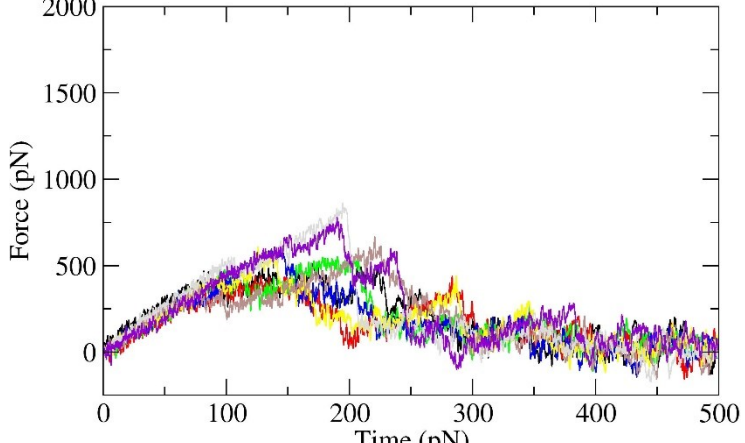
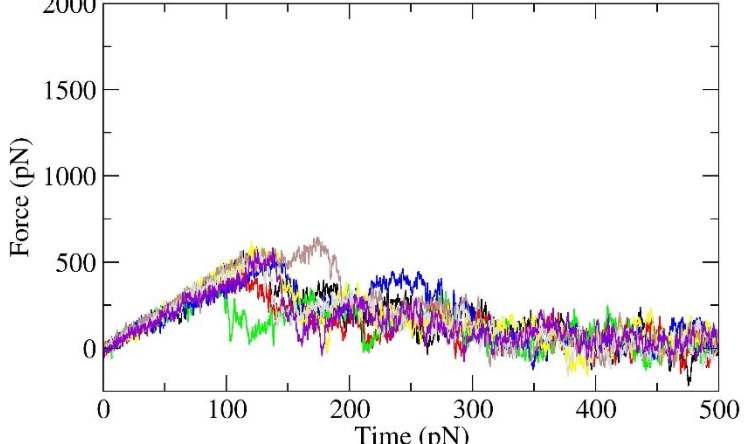
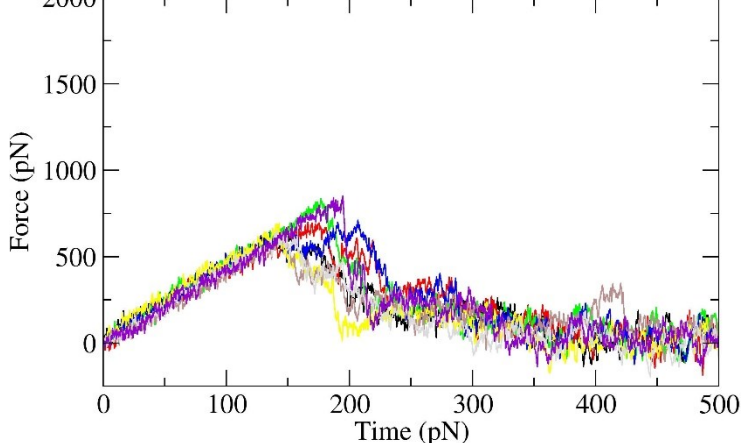


Table S3. The list of six top-lead marine compounds and FPL results.

N ^o	Compound	Pulling Work
1	48	
2	25	
3	40	

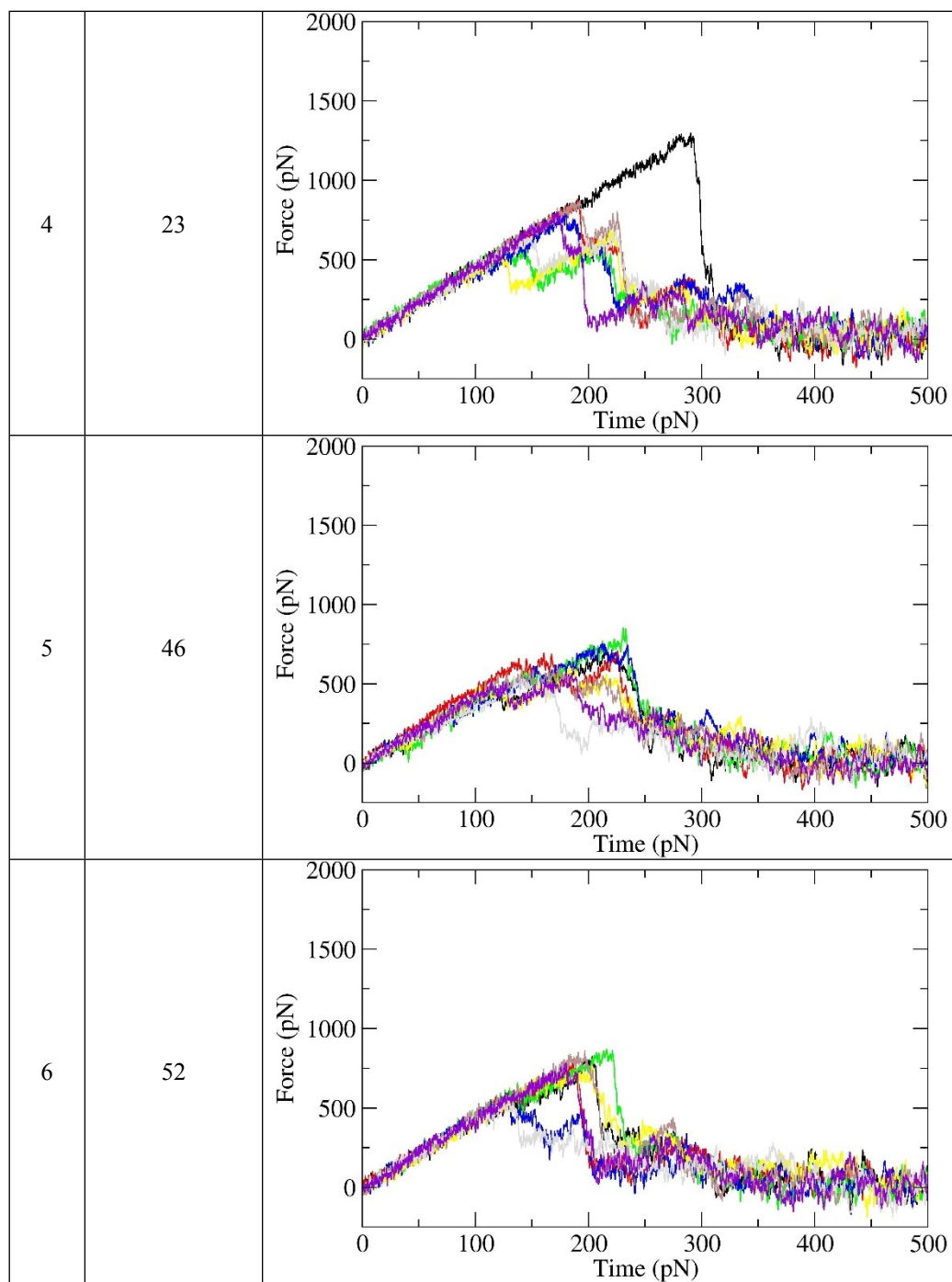
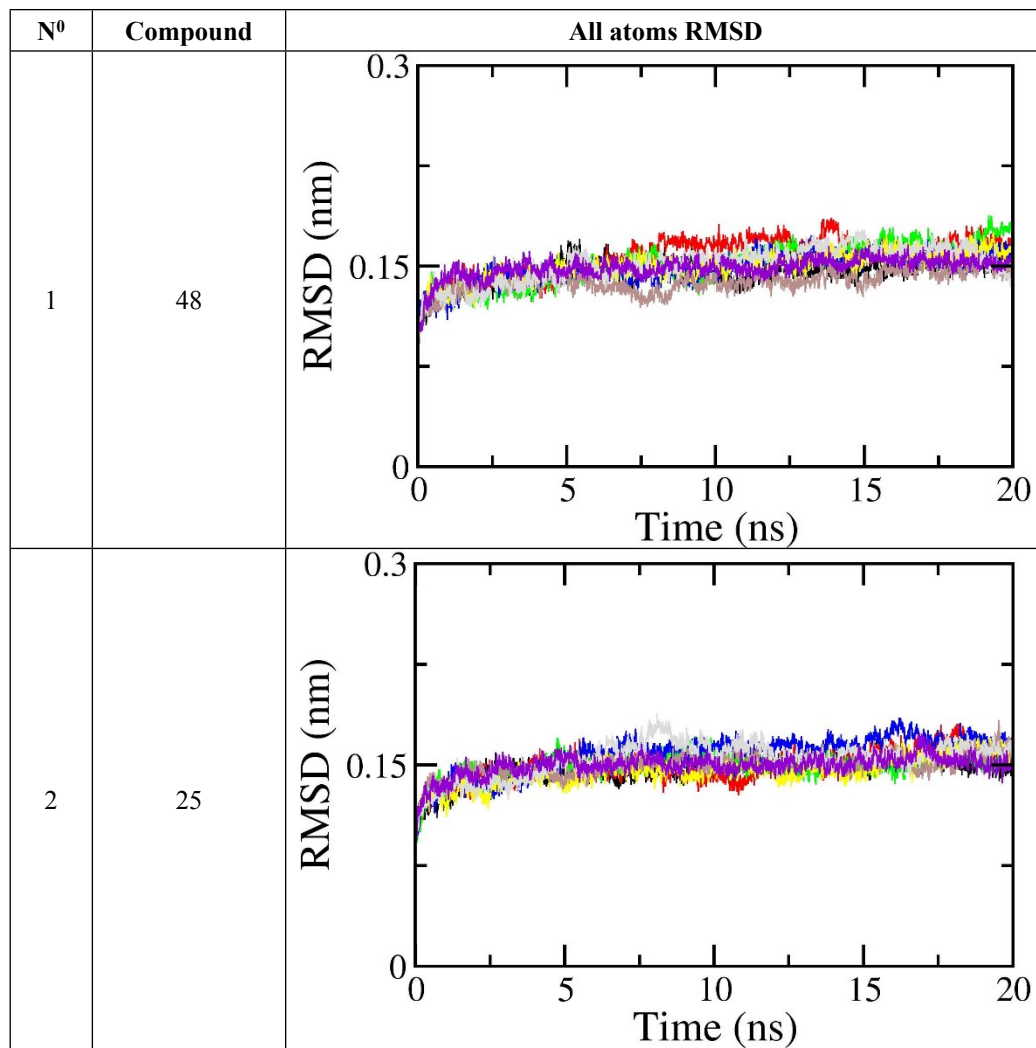
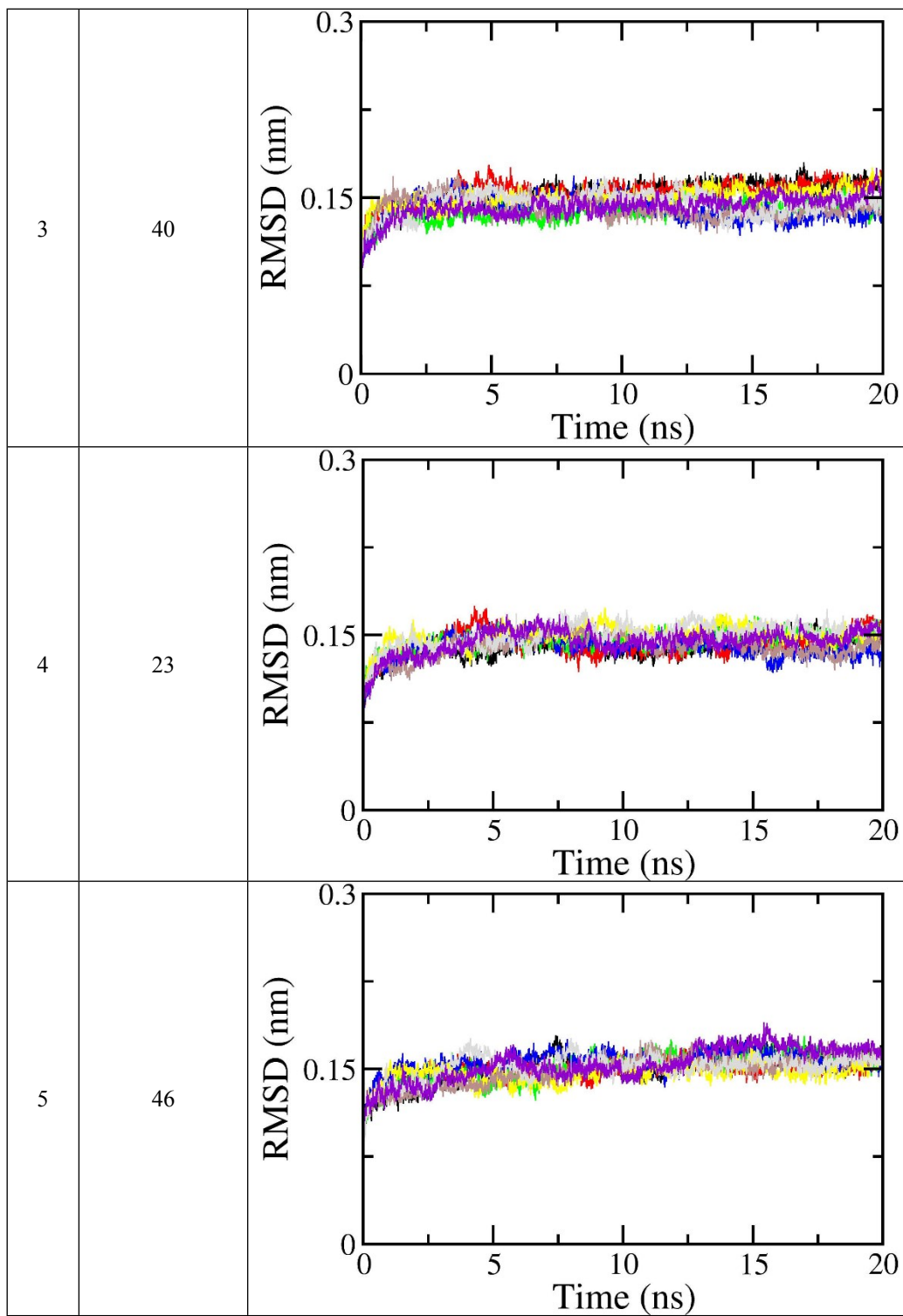


Table S4. All atom RMSD of Hsp90 + inhibitors over 8 independent MD trajectories with a length of 20 ns each.





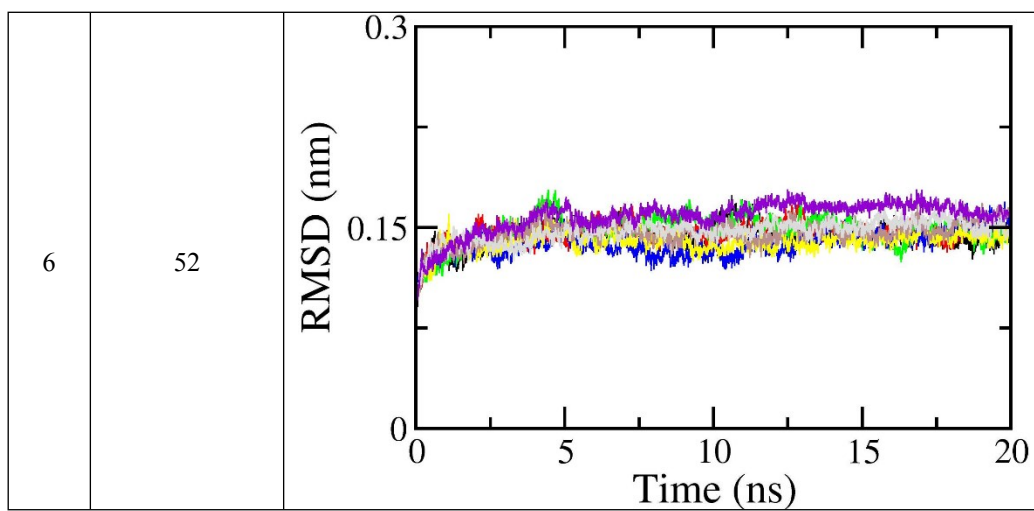
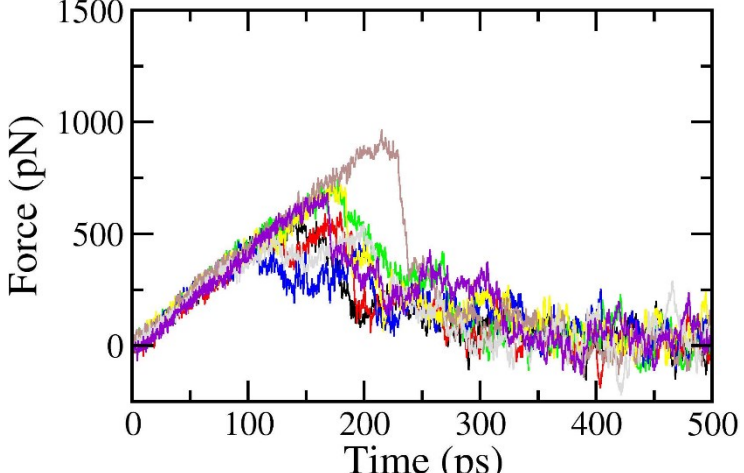
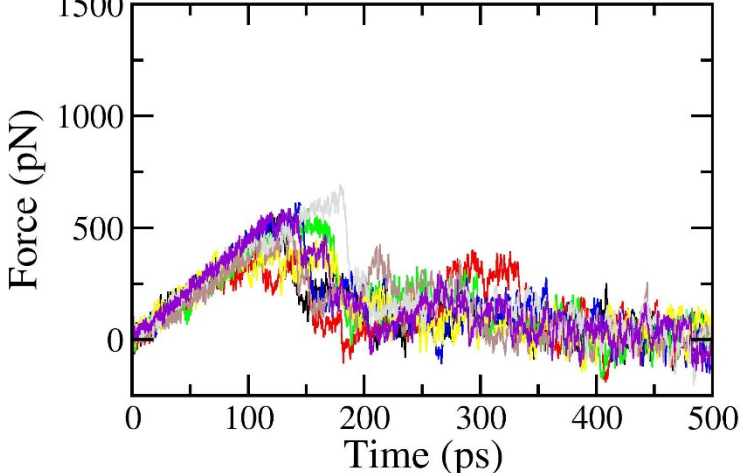
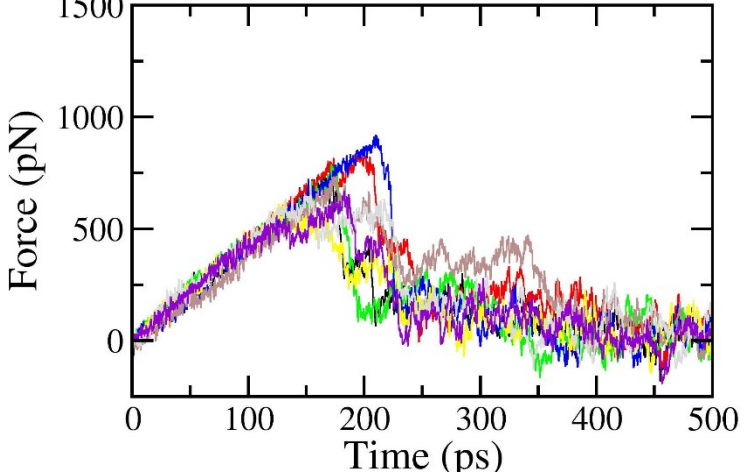


Table S5. The obtained values of the FPL calculations.

N^o	Name	F_{Max}^a	W^b
1	48	662.2 ± 49.3	71.0 ± 4.5
2	25	548.3 ± 30.7	56.2 ± 2.4
3	40	749.3 ± 32.1	81.2 ± 4.2
4	23	973.9 ± 76.0	108.1 ± 6.9
5	46	860.4 ± 59.0	95.0 ± 9.0
6	52	658.6 ± 45.4	63.5 ± 5.2

^aThe obtained value of the mean rupture force F_{Max} and ^bthe recorded metric of the pulling work W . The calculated error was the standard error of the average. The unit of force, energy, and inhibition constant is in pN, kcal mol⁻¹ and μM, respectively.

Table S6. The list of six top-lead marine compounds and FPL results.

N ^o	Compound	Pulling Work
1	48	 A line graph showing Force (pN) on the y-axis (0 to 1500) versus Time (ps) on the x-axis (0 to 500). Multiple colored lines represent individual pulling work trials. The force generally increases from 0 to a peak of approximately 800-1000 pN between 150 and 250 ps, then decreases and stabilizes around 200-500 pN for the remainder of the 500 ps duration.
2	25	 A line graph showing Force (pN) on the y-axis (0 to 1500) versus Time (ps) on the x-axis (0 to 500). Multiple colored lines represent individual pulling work trials. The force increases to a peak of approximately 500-700 pN between 100 and 200 ps, then decreases and stabilizes around 200-500 pN for the remainder of the 500 ps duration.
3	40	 A line graph showing Force (pN) on the y-axis (0 to 1500) versus Time (ps) on the x-axis (0 to 500). Multiple colored lines represent individual pulling work trials. The force increases to a peak of approximately 800-1000 pN between 150 and 250 ps, then decreases and stabilizes around 200-500 pN for the remainder of the 500 ps duration.

